

METHOD AND APPARATUS FOR DETERMINING MOLECULAR CRYSTAL STRUCTURES

Abstract of the disclosure

A method and apparatus for determining molecular crystal structures enables molecular crystal structures to be identified using only powder diffraction data. Trial crystal structures are reduced to a set of variables representative of the location and orientation of the molecule, torsion angles, bond lengths or bond angles. The experimental diffraction data provides a reduced representation of the data in the form of a structure factor intensity listing and covariance matrix. Trial structures are postulated and each is defined using the set of variables, which are used in determining a fitness of each trial structure with respect to the reduced representation of the experimental data. A crystal structure is output when the fitness value for the trial structure is less than or equal to a predetermined threshold. Identification of complex molecular crystal structures can be performed in seconds or minutes using conventional personal computers or workstations.